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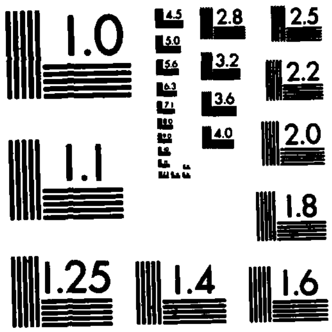

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This report summarizes results of the work on the contract to date in the areas of 2-D grid generation, 3-D grid generation, truncation error verification, 2-D adaptive grid for E-field calculations, and 3-D surface grid generation and interior grid control. The report also lists publications resulting from the contract work.

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AFOSR-TR- 82-1092

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15 October 1982

Major Carl Edward Oliver
AFOSR
Directorate of Mathematical and Information Sciences
Building 410
Bolling AFB, DC 20332

SUBJECT: FIRST RESEARCH PROGRESS AND FORECAST REPORT (10/15/82) FOR CONTRACT F49620-82-C-0064, "ADAPTIVE GRID GENERATION USING ELLIPTIC GENERATING EQUATIONS WITH PRECISE COORDINATE CONTROLS"

Dear Major Oliver:

This letter constitutes the required report on the subject contract, for the 5-month period from the inception of the contract on 15 May 1982.

Generally, I am extremely pleased with the progress accomplished and the forecast, detailed in the following topical areas.

(1) 2D GRID GENERATION

The codes for the generation of the 2D grid equations, the solution of the finite difference equations, and the verification process have all been successfully developed. See #2 below for details.

(2) 3D GRID GENERATION

We have completed development of codes for the transformation of general second-order equations in 3D into general nonorthogonal coordinates, for the solution of these equations by hopscotch SOR, for rigorously verifying the algebra and coding involved, for establishing the grid generation equations and solving them, and for rigorously verifying these.

Using Symbolic Manipulation* on a VAX computer, code was written to transform the general second-order PDE to general nonorthogonal coordinates. The result is a 19-point operator,

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*The Symbolic Manipulation work was done under related contract from the U.S. Army Research Office, and involved Dr. S. Steinberg.

since the 8 corner points on the cube of the 3D operator are identically zero. A Fortran subroutine was written to generate the 3D arrays for the finite difference coefficients. These were solved by hopscotch SOR code.

The validation procedure for the "hosted equations" (in this case, the variable-conductivity electric field equation) consisted of testing the truncation-error convergence of the solution. An inverse procedure was devised, in which the continuum solution was specified, chosen so as to possess enough structure to exercise all the derivatives of the operator and all finite-difference truncation errors. For the second-order operator and second-order accurate finite difference forms, the solution was specified as sol = $x^3y^4z^5$. The transformation used involved the hyperbolic tangent of the product of all three transformed coordinates, $\xi_i = x_i + \tanh(d_i xyz)$, where $x_1 \equiv x$, $x_2 \equiv y$, $x_3 \equiv z$. The hosted equation in the original coordinates was $L(\phi) \equiv \nabla \cdot \sigma \nabla \phi = q$. The variable conductivity σ was also chosen to give significant structure to the matrix, with $\sigma = \sigma_o \sin(xyz/x_{max}y_{max}z_{max})$. The non-homogeneous part q was chosen so as to give the desired solution, i.e. q = L(sol). This highly structured problem was then fed to the Symbolic Manipulation code, and the matrix problem generated by it was solved numerically. (In 2D, we used the GEM spatial marching codes, and in 3D, we used the hopscotch SOR solver.) By monitoring the truncation error as the grid was refined from 5^3, 9^3, 17^3, 33^3, we verified the transformation, the finite difference forms (validating the $O(\Delta^2)$ accuracy) and the iterative solution procedure. As expected theoretically, the value of $C = \Delta^2 \cdot TE$, where TE is the maximum truncation error in the mesh, becomes constant as the mesh is refined. The size of C depends on the grid stretching parameters d_i and σ_o, but the entire method remains $O(\Delta^2)$ accurate.

A similar procedure was followed for the grid generation equations themselves, although this was more complicated. A "solution" for the grid transformation problem $L(\xi_i) = P_i$ was chosen as $\xi_i = x_i + \tanh(D_i xyz)$, where the D_i are grid stretching parameters, not the same as the d_i used earlier. (Note the roles of x_i and ξ_i are reversed from the earlier case of the hosted equation validation.) The non-homogeneous terms P_i are then chosen to give the desired solution, $P_i = L(\xi_i)$ where L is the Laplacian in x,y,z. With ξ_i specified at each mesh point in the transformed domain, the x_i had to be obtained by solution of a 3x3 transcendental equation system. Because of round-off sensitivity (see below) this was accomplished with a 3x3 Newton-Raphson procedure, converged to essentially single precision on the computer. The numerical solution procedure for the grid generation equations was also more involved then the hosted equation solution, since it involved a nonlinear system of three coupled equations for x,y,z. This solution was obtained by outer (nonlinear) Picard iterations and inner (linear) hopscotch SOR solutions. The result and interpretation is the same as the hosted equation situation, with constancy of $C = \Delta^2 \cdot TE$ validating the transformation, the finite difference forms, and the solution procedure, with the grid varied from 5^3, 9^3, 17^3, 33^3.

The calculations were performed on a 32-bit computer, a VAX 780, with approximately 8 significant decimal figures of accuracy. The round-off problem only slightly obscured the truncation-error convergence testing for the hosted equations, but was a serious problem for the grid generation equations. A false indication of a persistent error, which stopped progress for the better part of a month, was eventually traced to the evaluation of the Laplacian of the solution, which involved three summations of terms containing sech^2 and tanh. We are still investigating the reason for the error, but it was cured, and the validation procedure was made successful, with a minor grouping of terms in the Laplacian subprogram.

Although this round-off error problem would have been nonexistent on a CDC or Cray computer, we are still convinced that the excellent interactive editing and running capabilities on the VAX computer was essential to the rapid development of these codes. In fact, the Symbolic Manipulation code used is available only on the VAX computers. However, even the other code components, involving more traditinal numerical methods, were developed much more rapidly than they would have been on a mainframe computer. We estimate a factor of 3 savings in code development time, with better structured code resulting also.

(3) TRUNCATION ERROR VERIFICATION

The question of the accuracy of grid transformation techniques has been confused recently. Mastin and others have gone through lengthy analyses and shown that second-order accuracy is lost for severe distortions. These analyses are in disagreement with previously published results, including some by the present P.I. Mastin has some experiments which he calls on to validate his results. The numerical experiments show that the truncation error increases as the grid distortion increases.

This work, and similar analyses, were the subject of private discussions at the Nashville conference on Grid Generation held in April 1982. I am of the opinion that these analyses are incorrect, and that the numerical experiments do not confirm or contradict the analysis. Everyone agrees that severe distortion will increase the truncation error, but the question of the order of the accuracy can only be settled by doing the kind of systematic truncation-error testing which we have done in the present work. The present results show clearly that second-order accuracy is maintained, even for strong grid distortion.

(4) 2D ADAPTIVE GRID FOR E-FIELD CALCULATIONS

A procedure and code has been successfully developed for solution-adaptive gridding for E-field calculations in 2D. The calculations are being performed, under separate funding, for the Air Force Weapons Laboratory in support of a laser development project. The solution-adaptive procedure was developed under present AFOSR funding.

This E-field calculation differs from most fluid dynamics calculations in that the maximum value of the electric field occurs on the boundary. (This is rigorously true for the linear case with constant conductivity, and is expected in all practical cases.) Thus, the grid adaptivity does not concern the grid point location at interior points, obtained with tailoring of the nonhomogeneous terms in the tranformation equations, but the location of the grid points on the boundary. This aspect of the grid transformation is also of interest to fluid dynamic calculations, however, and in fact has been largely neglected.

In previously published papers, the grid distribution along the boundaries has been obtained in an ad hoc manner, with no adaption used.

In the presently developed procedure, we obtain a first solution on a grid with the boundary distribution determined by the local curvature of the surface. (Default method consists of equidistribution of points over arc length, but this can be weighted to pack more points near local surface curvature. With the solution adaptive procedure, we find that equidistribution over arc length is adequate.) The second grid is obtained with boundary points packed more closely near the maximum E values, using an empirically-determined (user-specified) weighting factor. The process can be iterated to a convergence of the grid, but in practice a single adaptive step is sufficient to attain the increase in resolution desired.

Overall accuracy (e.g. in an L^2 norm on ϕ or E) is not the objective in this procedure, but rather the resolution of the maximum value of E. It is this maximum E which limits the power output of the laser, since it determines arcing. Although the first (non-adapted) grid may give E values which are quite accurate, say to 0.1%, the adaptive step increases the value of the maximum calculated E value by as much as 20% in geometries considered so far. It appears that this procedure can reduce the computing time to achieve a given level of resolution of maximum E by a factor of 2 to 5, compared to brute-force grid refinement.

Although conceptually simple, the implementation of this procedure involves a subtle procedure of what we have called "projective interpolation". The "true" or continuum surface is defined by a set of discrete coordinates and an associated interpolation rule; we refer to the discrete coordinate and the interpolation rule collectively as G_c. The initial grid G_1 is layed down by some rule, say the equidistribution in arc length, by reference to G_c, and is "on" G_c. But the discrete $y_\ell(x_\ell)$ differ; the domains of definition are not the same. For example, G_c may be defined by 1000 points and a cubic spline interpolation rule, whereas the initial grid G_1 might consist of 31 points on the boundary, none of which, other than the end-points, need correspond to any of the 1000 points of G_c. When the second (solution-adapted) grid G_2 is defined by resolution of the E-field, which has been calculated not on G_c but on G_1, the resulting grid points will be "on" G_1 (say, in the sense of being linear interpolants between points of G_1) but not generally "on" G_c. (This is true even if G_c was defined with a linear interpolation rule, as long as the defining points of G_c were not the first grid G_1. This is the only practical case to consider.) In order to assure that the solution adaptive grid is actually "on" G_c, a combination of interpolation and projection is necessary. This gets particularly tricky near acute angles in the boundary, which are not of practical interest in the laser electrodes but could be of interest in aerodynamics problems, where the analogous grid adaption would be motivated by the desire to accurately resolve separation/reattachment points. Even without the acute angle situation, the projective interpolation problem is difficult. The details of our "solution" will not be given here, but suffice it to say that the solution is heuristic. Note that when the interpolated function and the defining function have different domains of definition, we are out of the realm of analysis. (For example, their is no mean value theorem.)

We have given some consideration to the analogous 3D problem and have made some progress, but have not completed this work nor done any testing.

(5) 3D SURFACE GRID GENERATION AND INTERIOR GRID CONTROL

Aside from the solution-adaptive problem, and the associated projective interpolation problem mentioned above, the simple non-adaptive generation of the 3D grid on non-planar surfaces is a difficult problem. Ruppert of Boeing considers this the most difficult part of 3D aircraft calculations. P.D. Thomas has a good method which depends on projections from the aircraft boundary onto some outer surface. Although successful for a wide range of geometries, it will fail for difficult shapes where the projection is multivalued.

We have made some progress on a method of generating the surface grid using modified 3D grid generating equations solved in the non-planar surface. The concept would accomplish the surface grid generation in a smooth but otherwise general surface; e.g. $z_{surface}$ could be a multi-valued function of $x_{surface}$, $y_{surface}$. We have not advanced to the coding and testing stage as yet.

Likewise, we have not coded and tested the methods for internal grid point precise control. This will be addressed shortly, for the 2D problem first.

(6) PUBLICATIONS

We will present an invited paper entitled "Symbolic Manipulation and Computational Fluid Dynamics" at the AIAA Computational Fluid Dynamics Conference to be held July 1983 in the Boston area. The primary funding for this work was provided by the Army Research Office, but the paper will include much of the work done under the present AFOSR contract as well.

For the same meeting, I will be submitting a contributed paper on the adaptive surface gridding problem described above. If progress is rapid, I may also submit another paper on the 3D surface grid generation problem. Also, I will submit an Open Forum paper on the truncation-error validation problem, and try to lay to rest this question of the order of accuracy of highly distorted grids. This result would then be submitted to the AIAA JOURNAL as a Technical Note.

I have been invited to serve as the Editor for a Special Volume of COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING dedicated to Grid Generation. This issue will probably appear in early 1984.

(7) BUDGET

All expenditures, both direct charge and overhead items, are within the budget for this contract. We do not anticipate any changes in the expenditures or time allotments from the contract budget and SOW.

If further details are needed on any of these topics, please do not hesitate to contact me at the above address or telephone number.

Respectfully,

Patrick J. Roache

Dr. Patrick J. Roache, Prin. Inves.

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